Phase Behavior of Multiblock Polymers: Comparison of Theory and Experiments

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Introduction

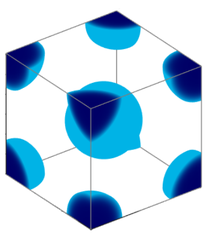
Block polymers self-assemble to form ordered structures at the nanometer scale. These nanostructures have many practical applications such as in computer chips, car tires, and adhesives [1,2]. The phase behavior of these materials can be studied using self-consistent field theory (SCFT). For this project, the open-source software package, Polymer Self-Consistent Field (PSCF) was used [3]. A critical parameter required to model these polymers using SCFT is the binary interaction parameter (χ) that measures the chemical incompatibility between monomers, and is inversely proportional to temperature.

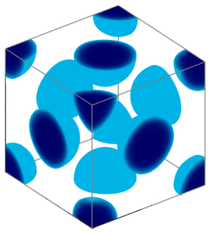
Scope

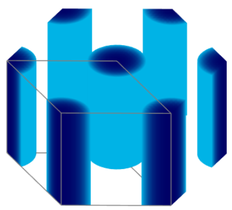
The goal of this project is to compare the experimentally observed phase behavior of a tetrablock terpolymer, poly [styrene-b-isoprene-b-styrene-b-ethylene oxide], (SISO) to that predicted by SCFT. Experimental data were fit to the results listed below, and consequently used to estimate each of the binary interaction parameters (χ_{IS}, χ_{IO}, and χ_{SO}).

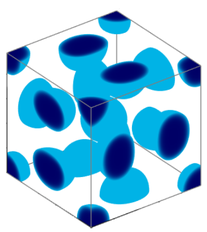
1: Mean - Field Theory [4].
2: Renormalized One-Loop (ROL) theory[5].
3: Rigorous Molecular Simulations [6].
4: Sensitivity Analysis.

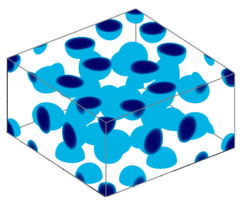
The free energies of various phases (shown in the diagram below) were calculated as a function of temperature for an experimentally studied tetrablock terpolymer molecule (SIS'O-0.73), reported by Chanpuriya et al. [7]. Each phase was modelled at increasing resolution until the free energy converged to at least seven decimal places. The phase behavior predicted by SCFT according to these parameters can be seen in the results section on the right.


Body-Centered Cubic (**BCC**)


Face-Centered Cubic (**FCC**)


Hexagonal-Cylinders (**Cyl**)


Frank-Kasper A15 (**A15**)


Frank-Kasper Sigma (**σ**)

Acknowledgements

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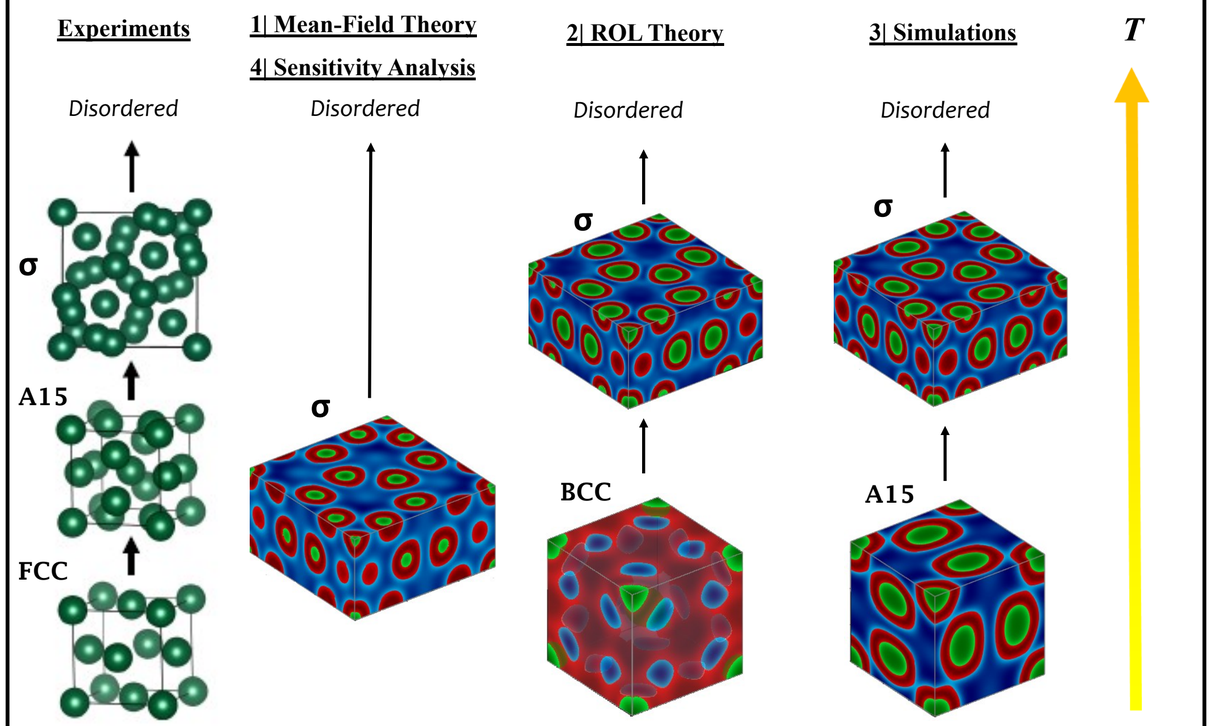
Results



Conclusion

All of the above methods predict the formation of the Frank-Kasper sigma phase before the system collapses into a disordered phase. In particular, using the parameters obtained by fitting experimental data to rigorous molecular simulations, SCFT was found to predict the formation of the A15 phase at a lower temperature , before the formation of the sigma phase, which is in agreement with the experimental results. Further investigation will be carried out at lower temperatures to determine if SCFT, using, these parameters , could predict the other structures seen in experiments. If the theoretical sequence agrees with the experimental sequence, then SCFT can be used to extensively model the phase behavior of SISO tetrablock terpolymers at varying block fractions.

References

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